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MRC Technical Summary Report #2202

RESONANCE THROUGH A STRICTLY SINGULAR PERTURBATION

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April 1981

(Received February 3, 1981)

Sponsored by

U. S. Army Research Office
P. O. Box 12211
Research Triangle Park
North Carolina 27709

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SIGNIFICANCE AND EXPLANATION

Unfortunately the usual definition of a resonant state, expressed in terms of the subsequent exponential decay, is not consistent with other necessary facts in the foundations of quantum theory, when most physical cases are considered. From the mathematical point of view the *resonance space* must be empty, which apparently is a poor physical result. The formal implications of this difficulty have been known for a long time.

Regardless of the improvement, made possible on the basis of measurement theory, this paper will be aiming at a redefinition, which maintains the plain conservative conception of the resonant state: It is supposed to constitute a unique, well defined initial condition for the time development of the physical system. If the description of the system is sufficiently complete under this condition, it motivates the use of strongly continuous semi-groups of contraction operators for the time development[1)]. In its generality the time development implies here the solution of the Schroedinger equation and the relevance to natural laws is therefore affirmed as well.

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1) Using Hadmard's criteria for a "well set" initial value problem [7] it was Phillips [8], who first used the initial state concept of mathematical physics to motivate the theory of semi-groups.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

UNIVERSITY OF WISCONSIN - MADISON
MATHEMATICS RESEARCH CENTER

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ABSTRACT

As a consequence of the formal difficulties in explaining resonances as solutions of the general Schroedinger equation, the procedure developed here exploits some fairly general properties of a semigroup, appropriate for the decay. A feature, which in this context may be named as "the paradox of resonance", will be analyzed to some extent. By generalizing the time development one can, however, formulate the resonant state in a consistent way. Its definition will be interpreted along the lines of strictly singular perturbations.

AMS (MOS) Subject Classifications: 81C05, 47A10, 47A55, 47D05

Key Words: Resonant state, extension of symmetric operators, strictly singular perturbation.

Work Unit Number 2 - Physical Mathematics

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Sponsored by the United States Army under Contract No. DAAG29-80-C-0041.

RESONANCE THROUGH A STRICTLY SINGULAR PERTURBATION

Ketill Ingólfsson*

1. Introduction.

When resonance is explained in the mathematical foundations of quantum theory, one usually presumes the observance of an eigenstate of a bound wave packet. The corresponding energy is in this case disclosed by the static central physical field. At first sight one would assume the existence of a state, in which no continuous spectrum is observed. In the very beginning of radiation theory, however, it was clearly explained [1] that this kind of energy does not exist and a resonant state is by observation never left alone by itself. The objectives of the theory were perturbed states and the determination of unperturbed states was highly ambiguous. Therefore it became customary to utilize in one way or the other the exponential time dependence of the decay, an experimentally very well established behaviour, in order to define the resonant state in the formal language of quantum physics.

The definition of the resonant state was, however, always considered as inconsistent. Already the pioneers of damping theory used to defend their results, although physically convincing [2], by assuming that the resonant development was in one way or the other a good approximation of the physical case. The investigation of the formal structure of deviations from the exponential decay brought until now detailed results [3], but has never contributed to a better understanding of the natural law. In order to answer the question, if formal resonance is relevant to natural laws, some authors have recently shown explicit calculations, which from a randomly repeated measurement allow a consistent redefinition of a resonant state[1)].

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1) See Ali, Fonda, Ghrirardi [4] and Fonda [5] for a review of the physical literture and Piron [6] on a recent mathematical analysis of the problem.

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These results will not be used directly for the form of resonance as it is presented in the following. The resonant decay may be interpreted as a suitable perturbation of a state, generated by a general wave equation with a self adjoint operator, with respect to which the subspace of absolute continuity is nonvanishing. According to a theorem of Weyl-von Neumann [9] there exists a perturbing term, self adjoint on a subspace and with sufficiently small Schmidt norm, such that the perturbed operator has a pure singular spectrum in the resonant subspace. By considering two strongly continuous one-parameter semi-groups of contraction operators one can present a pair of infinitesimal transformations generating asymptotically related semi-groups. The impossibility of interpreting in a great number of physical cases the resonant state from a natural exponential law, valid for all values of t on the nonnegative time-axis, will be referred to as the "paradox of resonance"[1]. The observance of this paradox shows that the perturbation series developed for the exponential decay can not be analytic in the coupling of the operators, when the corresponding perturbed states are defined in any neighborhood of $t = 0$. This fact can be confirmed by using a strictly singular perturbation of the operator[2]. Some technical problems of strictly singular perturbations series were already solved by the author in an earlier paper [12]. This approach may also be used for Gel'fand triples and intermediate spaces, as they are explained by Huet [13].

2. The paradox of resonance.

To start with one can use the following most general approach to the time development: A time dependent state is in quantum theory expressed in terms of a one-parameter unitary group. If ψ is a vector in the abstract Hilbert space and represents the state at some given instant, the physical situation can be explained t units of time later by the vector

1) The formal objections to this interpretation of the resonant state were discussed in Barry Simon's lecture at the 1978 SANIBEL meeting [10].

2) We are here quoting Seymour Goldberg's denotation of strictly compact cases [11].

(1) $$\psi_t = \exp(-iHt)\psi \quad .$$

According to a fundamental theorem of Stone [14] this vector is differentiable in the strong sense, if and only if it is of the domain of the infinitesimal generator of the group. The vector ψ_t is therefore considered as the solution of the generalized Schroedinger equation with the initial condition $\psi_0 = \psi$, when $\psi \in \mathcal{D}(H)$.

The following attempts to define the resonant state are based on the use of exponential behaviour of the decay, when it is generally described by the time development (1) with the self adjoint operator H defined in the general Hilbert space. A simple, widespread attempt is to use the

<u>Definition O</u> (fault): The vector ψ_γ with $\|\psi_\gamma\| = 1$ represents a resonant state of the width γ with respect to H, when the inequality

(2) $$|(\psi_\gamma, \exp(-iHt)\psi_\gamma)|^2 \leqq \exp(-\gamma t)$$

is fulfilled for all positive values of t. ■ The definition is *not consistent* with all terms entering this formulation. This is best seen by introducing for any $\psi_\gamma \in \mathcal{D}(H)$ with $\|\psi_\gamma\| = 1$ a real, even, time dependent function

(3) $$F_t = |(\psi_\gamma, \exp(-iHt)\psi_\gamma)|^2 \quad .$$

A function of this kind is continuously differentiable in any interval around o. For $t = o$ the value of F_t is 1 and the value of its derivative with respect to t is o. For enough small positive values of t one could find a contradiction to the statement (2) for any positive value of γ ("short time complaint"[1]).

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1) The notations "short time - " and the following "long time complaints" are quoted from Simon's lecture, loc.cit. [10].

One might try to circumnavigate this inconsistency by using the F_t as it is explained in (3) in more general terms as those expressed by the requirement (2). This leads to the

Definition OO (fault): The vector ψ_γ, which is a member of the subspace of singularity with respect to the self adjoint operator H, represents a resonant state, if the singular spectrum is not dense on the entire real line and the inequality

$$F_t \leq k \exp(-gt) \tag{4}$$

is for any g fulfilled for some k, when t is large enough. ∎ The formulation of this definition must be rejected because of the following inconsistency ("long time complaint"): The inner product $(\psi_\gamma, \exp(-iHt)\psi_\gamma)$ is the Fourier transform of a measure, which according to the Paley-Wiener theorem is at least analytic in a strip of the width g around the real line. On the other hand is the resolvent set $P(H_s)$ connected and there exists an open interval on the real line, on which the measure is zero. Therefore the measure is everywhere zero, the function F_t is identically zero in t and $\psi_\gamma = o$.

The explanation of the above inconsistency follows a similar description of the problem by Simon. In his "definition", however, semiboundedness is presupposed for the self adjoint operator H. In a recent paper of Ira Herbst [15] a physical case (the Stark effect) is discussed, in which the spectrum is absolutely continuous and covers the entire real line. In this case the "long time complaint" of Simon does not take effect, because H is not semibounded. The objection to the Definition OO, as it was explained before, can not be used either, because the subspace of singularity with respect to H is empty. The question one now tries to answer is, if there exists a modification of the former definition, for which an operator with the above described performance of the Herbst operator is applicable.

Definition OOO (fault): If the absolutely continuous spectrum of H, defined in a separable Hilbert space, is not empty and a bounded reduction of the operator exists, which defined onto an invariant subspace has a finite Schmidt norm, then is the vector ψ_γ of this separable Hilbert space a resonant state with respect to H, when the inequality (4) is fulfilled for any $g < \gamma$, some positive k and t large enough.■ One can show the impossibility of the inequality (4) in this definition, when t is large enough, through the following argumentation: Let $H = \int_{-\infty}^{\infty} \lambda dE(\lambda)$ be the spectral representation of H and $P = E(a) - E(b)$ for some $b < a$ the projection onto a subspace, which reduces H to a bounded operator with a finite Schmidt norm, $\|PH\|_2$. If the Hilbert space is separable, one can find $\{u_k\}$, *a dense subset* in the orthogonal complement to the above subspace. For each of these u_k there is a finite dimensional orthogonal projection, P_k, and a self adjoint operator Y_k with a finite Schmidt norm such that $\|(1 - P_k)u_k\| < \varepsilon$, $\|Y_k\|_2 < \varepsilon$ and $P_k(H + Y_k) \subset (H + Y_k)P_k$ for any ε (Lemma of von Neumann, loc.cit. [9]). The following, slightly modified version of the Weyl- von Neumann perturbation theorem is the consequence of the lemma in the above situation:

Theorem 1: Let H be a self adjoint operator in a separable Hilbert space with a nonvanishing absolutely continuous subspace with respect to H and let a bounded reduction of this H be of the Schmidt class. For any $\varepsilon > 0$ exist the numbers a and b with $b < a$ and a self adjoint operator A with the Schmidt norm less than ε such that $H + A$ has a pure point spectrum, which vanishes within (b,a).

The assumptions presupposed here imply that the absolutely continuous spectrum cannot cover $\mathbb{R}$ entirely. In a subspace determined by the projection operator $1 - E(a) + E(b)$ is A the operator, which in the Weyl- von Neumann theorem is stated as the perturbation of the energy operator to a spectrally singular operator. On the subspace determined by $E(a) - E(b)$ one can, however, take A as $-H$. The self adjoint perturbed operator $H + A$ is then pure singular and has not spectrum within (b,a). In accordance with F_t by (3) one can now define

(5) $$F'_t = |(\psi_\gamma, \exp(-i(H+A)t)\psi_\gamma)|^2 \ .$$

From the discussion of Definition OO it is obvious that F'_t can not fulfill an inequality like (4), when t is large enough. Let H' in the following mean $H + A$. By means of the Phillips equation[1)]

(6) $$(\psi_\gamma, \exp(-iHt)\psi_\gamma) = (\psi_\gamma, \exp(-iH't)\psi_\gamma) + (\exp(iH't)\psi_\gamma, \int_0^t ds \exp(iH's)(iA)\exp(-iHs)\psi_\gamma)$$

one can find the relation

(7) $$F'_t + F'^{\,1/2}_t \nabla'_t + F_t^{1/2} \nabla_t \Delta_t^{1/2} - F_t\Delta_t = o$$

with $\Delta_t = |(\psi_\gamma, \exp(iHt)\exp(-iH't)\psi_\gamma)|^2$ and $\{\nabla_t, \nabla'_t\}$ both real and bounded by the number

$$\sqrt{(1-F_t)(1-\Delta_t)} \leqq t \, \|A\|_2 \ .$$

If we claim that the inequality (4) is now true for F_t, the number $\|A\|_2$ can be chosen so small that the solution of (7) with respect to F'_t fulfills the inequality (4). As this is, however, not possible according to Theorem 1, the Definition OOO must be inconsistent.

The description of the inconsistencies in the Definitions O, OO and OOO has shown that the inequality (4) must not be used for the definition of the resonant state, if one of the following is true: The energy operator is semi-bounded, its resolvent set is connected or there exists an absolutely continuous spectrum although some reduction of the energy operator on the nonvanishing singular subspace has a finite Schmidt norm. There remains

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1) The name "Phillips equation" was suggested to the author by B. Simon.

the possibility of an absolutely continuous spectrum not fulfilling the above requirement for the Schmidt norm and a singular spectrum everywhere dense on the complement to the absolutely continuous spectrum with respect to the real line. It would obviously be useful, if some definition of the resonant state could be developed, which was applicable to more than these rare cases.

3. The resonant state.

In accordance with generalizations of Stone's theorem, which were originated in the semi-group theory of Hille and Yosida[1], the time development (1) can be replaced by a more general form. Let $\{Z(t); t \geq 0\}$ be a strongly continuous one-parameter semi-group of contraction operators defined on the general Hilbert space and G the infinitesimal generator of the semi-group. The time development of a vector, $\psi(t)$, which, analogous to (1), shows, how the state evolves from ψ, when $t \geq 0$, is now determined by the expression

(8) $$\psi(t) = Z(t)\psi \quad .$$

Similar to F_t, as it was defined by (3), one can then introduce a nonnegative form, $F(t)$, by

(9) $$F(t) = |(\psi, \psi(t))|^2$$

and include this form in relations demonstrating the mode of the decay. From here on the operator G generates a semi-group, $\zeta(\gamma)$, which by means of the expression (8) implies a decay effect for $\psi(t)$, characterized by the line breadth γ. This is generally the consequence on the following

[1] The theory, which Hille and Yosida proved independent of each other, is explained in Yosida's monograph [16].

Definition 1: A semi-group, $\{Z(t);t \geq 0\}$, is named a "decay group by the line breadth γ", denoted by $\zeta(\gamma)$, when the adjoint of the infinitesimal generator G is defined on an extension of the domain of G and when an operator, Ω, exists, fulfilling the following properties:

1) The numerical range of Ω is not the whole complex plane.

2) The domain of Ω is an extension of the domain of G and the closure of Ω is defined in the domain of Ω^*.

3) There exists a proper subspace, H_2, of the general Hilbert space, which reduces Ω such that H_1, the nonvanishing orthogonal complement to H_2, is the closure of the nullspace of Γ, which is here defined as $G - \Omega$, and the nullspace of G_1, which is the closure of the symmetric part of $G - \Gamma$.

4) The operator Γ is closable with the closure $c \cdot W$, where W is a partial isometry in the general Hilbert space mapping H_2 onto H_1 and $c \in ¢$.

5) If the closure of the skew symmetric part of G is denoted by G_0, then is

$$(\bar{\Gamma} + G_1)G_0 \subset G_0(\bar{\Gamma} + G_1) \quad . \tag{10}$$

6) If $z \in ¢$ with $\mathrm{Im} z \neq 0$ and $T = iG_0$, then is $\underset{\mathrm{Im}z>0}{\mathrm{def}(T-z)} = \underset{\mathrm{Im}z<0}{\mathrm{def}(T-z)}$.

7) The closure of the symmetric part of Ω has the negative eigenvalue $-\frac{\gamma}{2}$ with H_2 as the corresponding eigenspace. ■

This definition replaces the various attempts of section 2 to define a resonant state. It must be shown that the properties claimed under the definition imply a consistent structure. It is also important to know, which of its relevant terms are unique, when they exist. Because it is a infinitesimal generator, the operator G is closed and densely defined. An operator having these properties always fulfills the following: i) The adjoint of the operator is densely defined. ii) The adjoint of the adjoint is the original operator. Because $\mathcal{D}(\Gamma^+) \supset \mathcal{D}(G^+) \supset \mathcal{D}(G)$ one can use the decomposition

$$(11) \qquad G = \Gamma + \tfrac{1}{2}(G - \Gamma + G^+ - \Gamma^+) + \tfrac{1}{2}(G - \Gamma - G^+ + \Gamma^+)$$

of the infinitesimal generator, where the second term on the right is symmetric and the third term skew symmetric. The terms are not necessarily closed, because the reduction of G^+ onto $\mathcal{D}(G)$ is not always closed. The closures, G_1 and G_0, of these terms are again not necessarily self adjoint and skew self adjoint. If not, the property 6) will secure that they have self adjoint and skew self adjoint extensions [17].

From the property 1) follows that Ω is closable [18]. Any symmetric and skew symmetric extensions of the corresponding terms in (11) are on the forms $\tfrac{1}{2}(\Omega + \Omega^+)$ and $\tfrac{1}{2}(\Omega - \Omega^+)$ respectively, if and only if Ω also fulfills the property $\mathcal{D}(\Omega) \cap \mathcal{D}(\Omega^+) \supset \mathcal{D}(G)$. Their closures are therefore extensions of the operators G_1 and G_0. The operator G_0, which in this context corresponds to $-iH$ in the previous section, is bounded, if the numerical range of Ω if bounded, and semibounded, if the numerical range of Ω is bounded in the upper or the lower half-planes. The property 1) is therefore a proper generalization of the semi-boundedness, as it occured in the discussion on Definition OO in the previous section. The operators $\tfrac{1}{2}(\Omega + \Omega^+)$ and $\tfrac{1}{2}(\Omega - \Omega^+)$ are essentially self adjoint and skew self adjoint, if $\mathcal{D}(\bar{\Omega}) = \mathcal{D}(\Omega^+)$. The closures, $\tfrac{1}{2}(\bar{\Omega} + \Omega^+)$ and $\tfrac{1}{2}(\bar{\Omega} - \Omega^+)$ are then self adjoint and skew self adjoint. If conversely the closures of the expressions $\tfrac{1}{2}(\Omega + \Omega^+)$ or $\tfrac{1}{2}(\Omega - \Omega^+)$ are self adjoint or skew self adjoint respectively and the property 2) is fulfilled, then is $\mathcal{D}(\bar{\Omega}) = \mathcal{D}(\Omega^+)$[1]. One can therefore conclude from the property 7) that $\tfrac{1}{2}(\bar{\Omega} + \Omega^+)$ and $\tfrac{1}{2}(\bar{\Omega} - \Omega^+)$ are self adjoint and skew self adjoint extensions of G_1 and G_0 with the domain $\mathcal{D}(\bar{\Omega})$. The operator Γ is, when it exists, uniquely determined, because it is defined on the same domain as G. Being the nullspace of $\bar{\Gamma}$ the subspace H_1 is therefore uniquely determined. The closed and densely defined operators $\bar{\Gamma} + G_1$ and the self adjoint extension of G_0 fulfill the conditions for being infinitesimal generators of contraction semi-groups. (The condition

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1) This follows from the following: If an operator, A, is closed and densely defined in a separable Hilbert space, $\hat{A}$ is a closed extension of A and $A^+ = \hat{A}^+$, then is $A = \hat{A}$.

concerning the bounds of both resolvents [16] is fulfilled through the symmetry and skew symmetry.) The semi-groups, which they generate, will be denoted by $\{Z_0(t); t \geq 0\}$ and $\{Z_1(t); t \geq 0\}$ respectively. The operators $\{Z_0(t)\}$ are, when reduced by the subspaces H_1 and H_2, unitary on these spaces for any positive value of t[1]. The state vector (1) is a special case of the time development by (8), when H_2 vanishes and the skew symmetric part of Ω is skew self adjoint. In the following we will, however, consider H_2 as a non empty space and H_1 a proper subspace of the general Hilbert space. The resonant state may now be defined by the

<u>Definition 2</u>: If G is the infinitesimal generator of a decay group, $\zeta(\gamma)$, in accordance with Definition 1, the vector ψ_γ is a resonant state with respect to the line breadth γ when $\psi_\gamma \in \mathcal{D}(G)$. ■ If H_2 is not empty, $\psi_\gamma \in H_2 \cap \mathcal{D}(G)$ and $Z(t) \in \zeta(\gamma)$, we can compute $\psi(t)$ by using the properties implied by the Definition 1. This shows that

$$(12) \qquad \psi(t) = \exp(-\tfrac{\gamma}{2}\,t)Z_0(t)\psi_\gamma + (1-\exp(-\tfrac{\gamma}{2}\,t)) \cdot Z_0(t)\,\frac{2c}{\gamma}\,W\psi_\gamma \quad .$$

From this equation follows that $F(t) \leq \exp(-\gamma t)$ for all nonnegative t. Using the semi-group properties one can show that this inequality is true, if $\psi_\gamma = Z(s)\psi_2$ with s some positive number and $\psi_2 \in H_2 \cap \mathcal{D}(G)$ being different from 0. It would, however, be possible, on the same reasons as the objection to Definition 0, to prove that $F(t)$ is larger than $\exp(-\gamma t)$ for $\psi_\gamma \in H_1 \cap \mathcal{D}(G_0)$ and t small enough. The generalization of the inequality (2) is therefore not possible for all nonnegative values of t and any $\psi \in \mathcal{D}(G)$. Using the linearity of the semigroups one can, however, show that the generalization of the inequality (4),

$$F(t) \leq k\,\exp(-gt) \quad ,$$

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1) This follows from a theorem characterizing the generators of isometric semi-groups, which is a simple generalization of Stone's theorem on unitary groups [12].

is fulfilled for any t large enough. For the derivation of this inequality we have also used the fact that the ranges of the unitary $\{Z_0(t)\}$ are contained in the domain of G.

This result may be interpreted in the following way in terms of the concepts discussed in the previous section: If the self adjoint extension of iG_0, considered above, is the operator entering the Schroedinger equation for a spontaneous decay, when described in the Hilbert space $\mathcal{H}_1$, one can extend the space and assume the existence of $\mathcal{H}_2$, a subspace orthogonal to $\mathcal{H}_1$. $F(t)$ with $\psi_\gamma \in \mathcal{D}(G) \cap \mathcal{H}_1$ is even still fulfilling the above inequality, when t is large enough. The only difference to the situation in the previous section is then that the time development can be written as a linear combination of terms as (8) in the general Hilbert space, and $\psi_\gamma \in \mathcal{D}(G)$ may be a restriction to the choice of the initial state.

4. <u>The perturbation series.</u> When one now has arrived at a suitable definition of the resonant state, how can it be used in a practical case? In a previous paper [12] the author discussed a series,

$$Z(t)\psi = \sum_{0}^{n-1} A_\nu(t)\psi + R_n(t)\psi \quad , \tag{13}$$

where the terms $A_\nu(t)\psi$ are determined by the recurrence relations

$$A_\nu(t)\psi = -iU^o(t)\int_0^t ds\; U^o(s)^+\, V\, A_{\nu-1}(s) \qquad \nu \geq 1$$

$$A_o(t)\psi = U^o(t)\psi$$

and the remainder term $R_n(t)\psi$ obeys for $n \geq 1$ a similar relation with $R_0(t)$ being $Z(t)$. Then is

$$R_n(t)\psi = A_n(t)\psi + R_{n+1}(t)\psi \tag{14}$$

and for $n = 0$ this is just the Phillips equation (6), when we take the inner product by ψ. The series converges asymptotically according to the estimate

$$\|R_n(t)\psi\| \leq t\, M \sup_{s<t} \left(\|R_{n-1}(s)\psi\| + \|H^O R_{n-1}(s)\psi\| \right) , \tag{15}$$

if V is H^O-strictly singular and $\psi \in \mathcal{D}(G)$. In this series is iH^O the generator of the unitary group $\{U^O(t)\}$.

Let us now look back to our original problem, the spontaneous decay. We may find a self adjoint operator (the self adjoint extension of $-iG_0$ on $\mathcal{D}(G)$) in some Hilbert space (i.e. $\mathcal{H}_1$). We have constructed a larger space and a partial isometry between the spaces (i.e. the operator W). There exists a decay group in the large space, which on the smaller space is unitary. The decay can be described as an asymptotically converging series according to (13) and (15). The remainder term $R_1(t)\psi$, achieved by applying an iteration of (14) in as many terms as one likes, is the deviation from the exponential decay. The reduction $\mathcal{D}(G) \downharpoonright \mathcal{H}_1$ represents the resonant subspace.

When the physicists claim, as they have been doing the last 15 years, that the deviations from the exponential decay have no meaning for the description of nature, they are in fact right. The above formulation might tell why. The deviation is originated in an extension of the physical *space* and therefore not relevant to the physical law. This conclusion is independent on the way the series (13) converges. We have, however, chosen by G a general possibility to conceive the remainder term, which fulfills the purpose of asymptotic series.

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER #2202	2. GOVT ACCESSION NO. AD-A100 605	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) RESONANCE THROUGH A STRICTLY SINGULAR PERTURBATION		5. TYPE OF REPORT & PERIOD COVERED Summary Report - no specific reporting period
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Ketill Ingólfsson		8. CONTRACT OR GRANT NUMBER(s) DAAG29-80-C-0041
9. PERFORMING ORGANIZATION NAME AND ADDRESS Mathematics Research Center, University of Wisconsin 610 Walnut Street Madison, Wisconsin 53706		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Work Unit Number 2 - Physical Mathematics
11. CONTROLLING OFFICE NAME AND ADDRESS U. S. Army Research Office P.O. Box 12211 Research Triangle Park, North Carolina 27709		12. REPORT DATE April 1981
		13. NUMBER OF PAGES 13
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Resonant state, extension of symmetric operators, strictly singular perturbation

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

As a consequence of the formal difficulties in explaining resonances as solutions of the general Schroedinger equation, the procedure developed here exploits some fairly general properties of a semigroup, appropriate for the decay. A feature, which in this context may be named as "the paradox of resonance", will be analyzed to some extent. By generalizing the time development one can, however, formulate the resonant state in a consistent way. Its definition will be interpreted along the lines of strictly singular perturbations.